

Structure 1a

=> fil reg
FILE 'REGISTRY' ENTERED AT 09:24:05 ON 19 SEP 2002
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provided by InfoChem.

STRUCTURE FILE UPDATES: 17 SEP 2002 HIGHEST RN 452274-20-3
DICTIONARY FILE UPDATES: 17 SEP 2002 HIGHEST RN 452274-20-3

TSCA INFORMATION NOW CURRENT THROUGH MAY 20, 2002

Please note that search-term pricing does apply when
conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. See HELP
PROPERTIES for more information. See STNote 27, Searching Properties
in the CAS Registry File, for complete details:
<http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf>

=> d his

(FILE 'HCAPLUS' ENTERED AT 09:19:37 ON 19 SEP 2002)
DEL HIS Y

FILE 'REGISTRY' ENTERED AT 09:23:58 ON 19 SEP 2002

FILE 'REGISTRY' ENTERED AT 09:24:05 ON 19 SEP 2002

=> d que stat
NO L# DEFINED

=> fil reg
FILE 'REGISTRY' ENTERED AT 09:24:21 ON 19 SEP 2002
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provided by InfoChem.

STRUCTURE FILE UPDATES: 17 SEP 2002 HIGHEST RN 452274-20-3
DICTIONARY FILE UPDATES: 17 SEP 2002 HIGHEST RN 452274-20-3

TSCA INFORMATION NOW CURRENT THROUGH MAY 20, 2002

Please note that search-term pricing does apply when
conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. See HELP
PROPERTIES for more information. See STNote 27, Searching Properties
in the CAS Registry File, for complete details:
<http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf>

=> d his

(FILE 'HCAPLUS' ENTERED AT 09:19:37 ON 19 SEP 2002)
DEL HIS Y

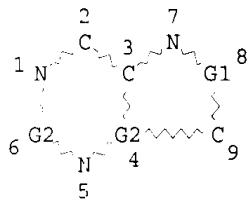
FILE 'REGISTRY' ENTERED AT 09:23:58 ON 19 SEP 2002

FILE 'REGISTRY' ENTERED AT 09:24:05 ON 19 SEP 2002
ACT ONEA/A

L1 STR
L2 (6184)SEA FILE=REGISTRY SSS FUL L1 - cover all structure 1~6.
L3 STR
L4 17 SEA FILE=REGISTRY SUB=L2 SSS FUL L3 - cover ^ 1a

FILE 'REGISTRY' ENTERED AT 09:24:21 ON 19 SEP 2002

=> d que stat 14
L1 STR



VAR G1=C/N/O/S

VAR G2=C/N

NODE ATTRIBUTES:

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

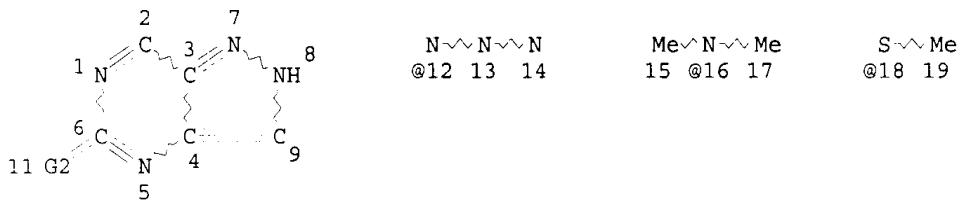
RSPEC I

NUMBER OF NODES IS 9

STEREO ATTRIBUTES: NONE

L2 (6184)SEA FILE=REGISTRY SSS FUL L1

L3 STR



VAR G2=H/NH2/16/12/F/CN/OME/18/SH/OH/CL/NO2/CF3/ME/ET

NODE ATTRIBUTES:

CONNECT IS E3 RC AT 9

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RSPEC I

Crane 09/526,348

NUMBER OF NODES IS 18

STEREO ATTRIBUTES: NONE

L4 17 SEA FILE=REGISTRY SUB=L2 SSS FUL L3

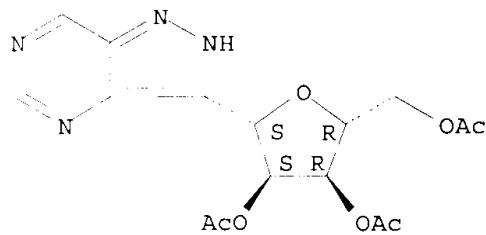
100.0% PROCESSED 3644 ITERATIONS
SEARCH TIME: 00.00.01

17 ANSWERS

=> d l4 ide can 1-17

L4 ANSWER 1 OF 17 REGISTRY COPYRIGHT 2002 ACS
RN 291536-72-6 REGISTRY
CN D-Ribitol, 1,4-anhydro-1-C-2H-pyrazolo[4,3-d]pyrimidin-3-yl-,
2,3,5-triacetate, (1S)- (9CI) (CA INDEX NAME)
PS STEREOSEARCH
MF C16 H18 N4 O7
SR CA
LC STN Files: CA, CAPLUS

Absolute stereochemistry.

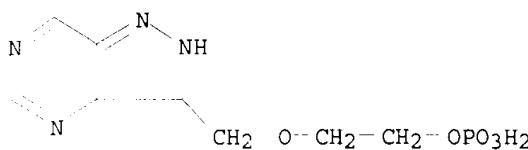


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 133:222974

L4 ANSWER 2 OF 17 REGISTRY COPYRIGHT 2002 ACS
RN 291536-71-5 REGISTRY
CN Ethanol, 2-(2H-pyrazolo[4,3-d]pyrimidin-3-ylmethoxy)-, dihydrogen phosphate (ester), disodium salt (9CI) (CA INDEX NAME)
MF C8 H11 N4 O5 P . 2 Na
SR CA
LC STN Files: CA, CAPLUS

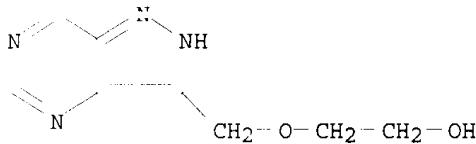


● 2 Na

1 REFERENCES IN FILE CA (1967 TO DATE)
 1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 133:222974

L4 ANSWER 3 OF 17 REGISTRY COPYRIGHT 2002 ACS
 RN 291536-70-4 REGISTRY
 CN Ethanol, 2-(2H-pyrazolo[4,3-d]pyrimidin-3-ylmethoxy)- (9CI) (CA INDEX NAME)
 FS 3D CONCORD
 MF C8 H10 N4 O2
 SR CA
 LC STN Files: CA, CAPLUS



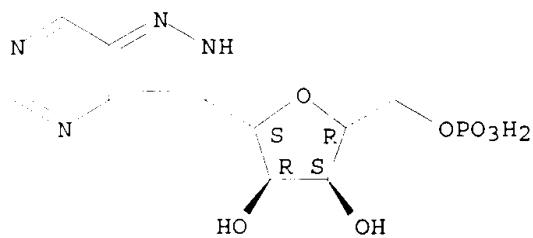
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
 1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 133:222974

L4 ANSWER 4 OF 17 REGISTRY COPYRIGHT 2002 ACS
 RN 291536-69-1 REGISTRY
 CN D-Ribitol, 1,4-anhydro-1-C-2H-pyrazolo[4,3-d]pyrimidin-3-yl-, 5-(dihydrogen phosphate), disodium salt (9CI) (CA INDEX NAME)
 FS STEREOSEARCH
 MF C10 H13 N4 O7 P . 2 Na
 SR CA
 LC STN Files: CA, CAPLUS

Absolute stereochemistry.



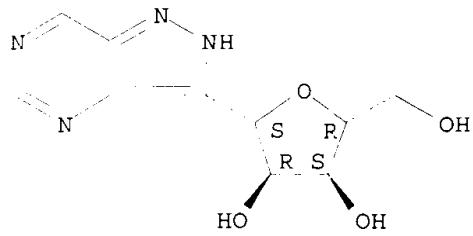
● 2 Na

1 REFERENCES IN FILE CA (1967 TO DATE)
 1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 133:222974

L4 ANSWER 5 OF 17 REGISTRY COPYRIGHT 2002 ACS
 RN 291536-67-9 REGISTRY
 CN D-Ribitol, 1,4-anhydro-1-C-2H-pyrazolo[4,3-d]pyrimidin-3-yl-, (1S)- (9CI)
 (CA INDEX NAME)
 FS STEREOSEARCH
 MF C10 H12 N4 O4
 SR CA
 LC STN Files: CA, CAPLUS

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1967 TO DATE)
 2 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 134:237749

REFERENCE 2: 133:222974

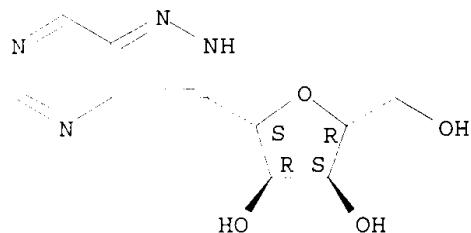
L4 ANSWER 6 OF 17 REGISTRY COPYRIGHT 2002 ACS
 RN 123238-52-8 REGISTRY
 CN D-Ribitol, 1-C-(7-amino-2H-pyrazolo[4,3-d]pyrimidin-3-yl)-1,4-anhydro-,
 conjugate monoacid, (1S)- (9CI) (CA INDEX NAME)
 OTHER CA INDEX NAMES:
 CN 2H-Pyrazolo[4,3-d]pyrimidine, D-ribitol deriv.
 FS STEREOSEARCH

Crane 09/526, 348

MF C10 H13 N5 O4 . H
SR CA
LC STN Files: CA, CAPLUS
CRN (57101-52-7)

Absolute stereochemistry.

NH₂



H⁺

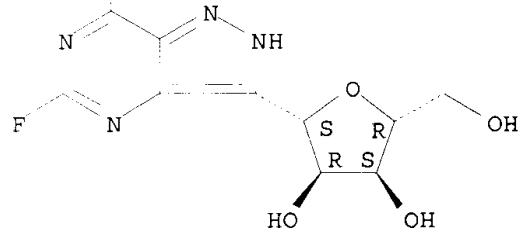
1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 111:166765

ANSWER / OR 1/ REGISTRY COPYRIGHT 2002 ACS
RN 123162-34-5 REGISTRY
CN D-Ribitol, 1-C-(7-amino-5-fluoro-2H-pyrazolo[4,3-d]pyrimidin-3-yl)-1,4-anhydro-, (1S)- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 2H-Pyrazolo[4,3-d]pyrimidine, D-ribitol deriv.
FS STEREOSEARCH
MF C10 H12 F N5 O4
SR CA
LC STN Files: CA, CAPLUS

Absolute stereochemistry.

NH₂



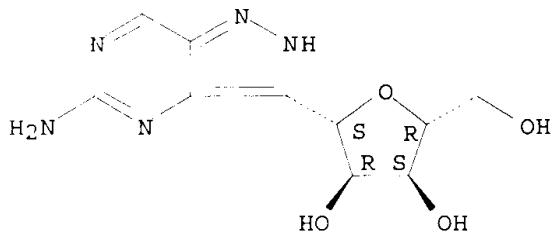
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 111:166765

L4 ANSWER 8 OF 17 REGISTRY COPYRIGHT 2002 ACS
 RN 123162-33-4 REGISTRY
 CN D-Ribitol, 1,4-anhydro-1-C-(5,7-diamino-2H-pyrazolo[4,3-d]pyrimidin-3-yl)-
 ,(1S)- (9CI) (CA INDEX NAME)
 OTHER CA INDEX NAMES:
 CN 2H-Pyrazolo[4,3-d]pyrimidine, D-ribitol deriv.
 FS STEREOSEARCH
 MF C10 H14 N6 O4
 SR CA
 LC STN Files: CA, CAPLUS

Absolute stereochemistry.

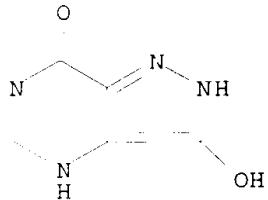
NH₂

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
 1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 111:166765

L4 ANSWER 9 OF 17 REGISTRY COPYRIGHT 2002 ACS
 RN 87499-14-7 REGISTRY
 CN 7H-Pyrazolo[4,3-d]pyrimidin-7-one, 2,4-dihydro-3-hydroxy- (9CI) (CA INDEX
 NAME)
 FS 3D CONCORD
 MF C5 H4 N4 O2
 LC STN Files: BEILSTEIN*, CA, CAPLUS
 (*File contains numerically searchable property data)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

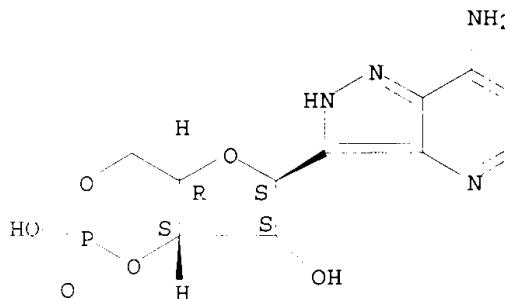
Crane 09/526, 348

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 99:158362

L4 ANSWER 10 OF 17 REGISTRY COPYRIGHT 2002 ACS
RN 71972-01-5 REGISTRY
CN D-Ribitol, 1-C-(7-amino-2H-pyrazolo[4,3-d]pyrimidin-3-yl)-1,4-anhydro-,
cyclic 3,5-(hydrogen phosphate), (S)- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 2H-Pyrazolo[4,3-d]pyrimidine, D-ribitol deriv.
CN 4H-Furo[3,2-d]-1,3,2-dioxaphosphorin, D-ribitol deriv.
FS STEREOSEARCH
MF C10 H12 N5 O6 P
LC STN Files: CA, CAPLUS

Absolute stereochemistry.

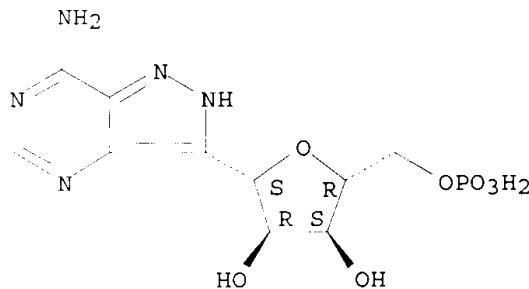


1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 91:211773

L4 ANSWER 11 OF 17 REGISTRY COPYRIGHT 2002 ACS
RN 71972-00-4 REGISTRY
CN D-Ribitol, 1-C-(7-amino-2H-pyrazolo[4,3-d]pyrimidin-3-yl)-1,4-anhydro-,
5-(dihydrogen phosphate), (S)- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 2H-Pyrazolo[4,3-d]pyrimidine, D-ribitol deriv.
FS STEREOSEARCH
MF C10 H14 N5 O7 P
LC STN Files: CA, CAPLUS

Absolute stereochemistry.



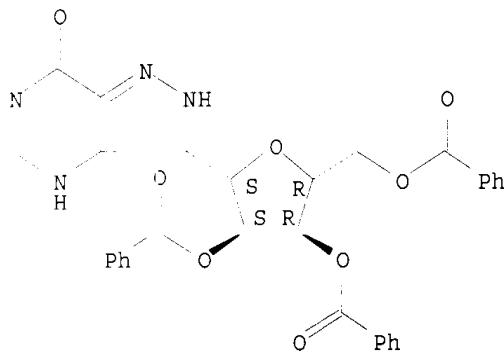
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 91:211773

L4 ANSWER 12 OF 17 REGISTRY COPYRIGHT 2002 ACS
RN 67560-82-1 REGISTRY
CN 7H-Pyrazolo[4,3-d]pyrimidin-7-one, 2,4-dihydro-3-(2,3,5-tri-O-benzoyl-.beta.-D-ribofuranosyl)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C31 H24 N4 O8
LC STN Files: BEILSTEIN*, CA, CAPLUS
(*File contains numerically searchable property data)

Absolute stereochemistry.



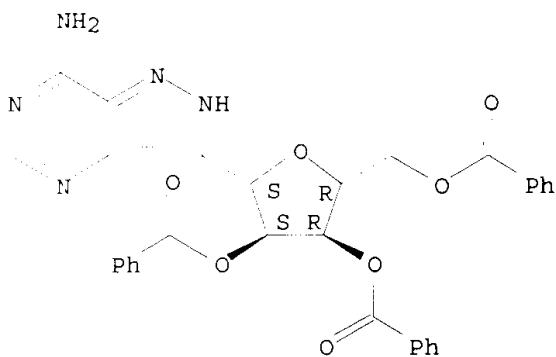
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 89:197857

L4 ANSWER 13 OF 17 REGISTRY COPYRIGHT 2002 ACS
RN 67560-80-9 REGISTRY
CN D-Ribitol, 1-C-(7-amino-2H-pyrazolo[4,3-d]pyrimidin-3-yl)-1,4-anhydro-, 2,3,5-tribenzoate, (S)- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 2H-Pyrazolo[4,3-d]pyrimidine, D-ribitol deriv.
FS STEREOSEARCH
MF C31 H25 N5 O7
LC STN Files: BEILSTEIN*, CA, CAPLUS
(*File contains numerically searchable property data)

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

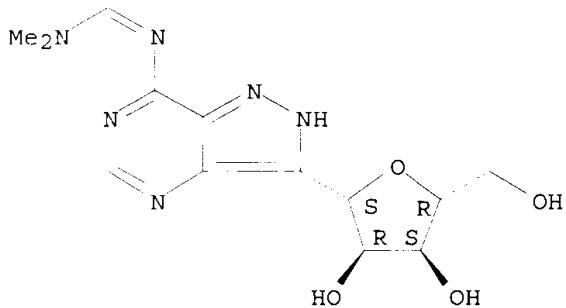
1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 89:197857

L4 ANSWER 14 OF 17 REGISTRY COPYRIGHT 2002 ACS
 RN 63358-78-1 REGISTRY
 CN Methanimidamide, N,N-dimethyl-N'-(3-.beta.-D-ribofuranosyl-2H-pyrazolo[4,3-d]pyrimidin-7-yl)- (9CI) (CA INDEX NAME)
 OTHER CA INDEX NAMES:
 LN 2H-Pyrazolo[4,3-d]pyrimidine, methanimidamide deriv.
 FS STEREOSEARCH
 MF C13 H18 N6 O4
 LC STN Files: BEILSTEIN*, CA, CAPLUS
 (*File contains numerically searchable property data)

Absolute stereochemistry.

Double bond geometry unknown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

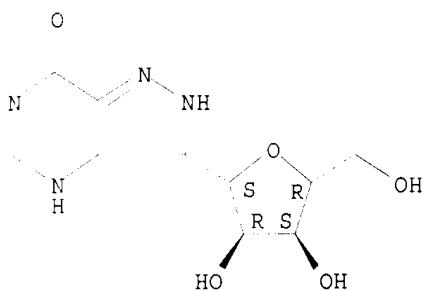
1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 87:68560

L4 ANSWER 15 OF 17 REGISTRY COPYRIGHT 2002 ACS

RN 63347-44-4 REGISTRY
CN 7H-Pyrazolo[4,3-d]pyrimidin-7-one, 2,4-dihydro-3-.beta.-D-ribofuranosyl-
(9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C10 H12 N4 O5
LC STN Files: BEILSTEIN*, CA, CAPLUS
(*File contains numerically searchable property data)

Absolute stereochemistry.



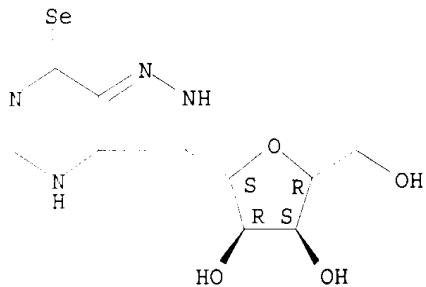
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 87:68560

L4 ANSWER 16 OF 17 REGISTRY COPYRIGHT 2002 ACS
RN 57101-53-8 REGISTRY
CN 7H-Pyrazolo[4,3-d]pyrimidine-7-selone, 2,4-dihydro-3-.beta.-D-
ribofuranosyl- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C10 H12 N4 O4 Se
LC STN Files: CA, CAPLUS

Absolute stereochemistry.



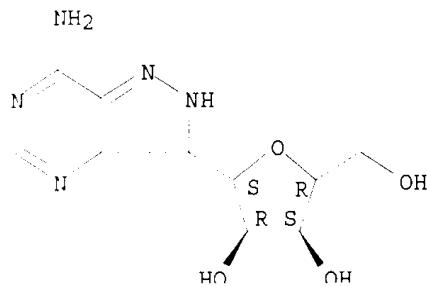
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 83:97797

L4 ANSWER 17 OF 17 REGISTRY COPYRIGHT 2002 ACS
 FN 57101-52-7 REGISTRY
 CN D-Ribitol, 1-C-(7-amino-2H-pyrazolo[4,3-d]pyrimidin-3-yl)-1,4-anhydro-,
 (S)- (9CI) (CA INDEX NAME)
 OTHER CA INDEX NAMES:
 CN 2H-Pyrazolo[4,3-d]pyrimidine, D-ribitol deriv.
 OTHER NAMES:
 CN 2H-Formycin
 FS STEREOSEARCH
 MF C10 H13 N5 O4
 CI COM
 LC STN Files: BEILSTEIN*, CA, CAPLUS
 (*File contains numerically searchable property data)

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

7 REFERENCES IN FILE CA (1967 TO DATE)
 7 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 121:83847

REFERENCE 2: 112:212992

REFERENCE 3: 111:166765

REFERENCE 4: 93:113653

REFERENCE 5: 89:110233

REFERENCE 6: 87:68560

REFERENCE 7: 83:97797

=> fil hcaplus
 FILE 'HCAPLUS' ENTERED AT 09:24:41 ON 19 SEP 2002
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FILE COVERS 1907 - 19 Sep 2002 VOL 137 ISS 12
FILE LAST UPDATED: 18 Sep 2002 (20020918/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

CAS roles have been modified effective December 16, 2001. Please check your SDI profiles to see if they need to be revised. For information on CAS roles, enter HELP ROLES at an arrow prompt or use the CAS Roles thesaurus (/RL field) in this file.

'OBI' IS DEFAULT SEARCH FIELD FOR 'HCAPLUS' FILE

=> S 14
L5 12 L4

=> d .ca hitstr 15 1-12]
~~1-12] IS NOT A VALID FORMAT FOR FILE 'HCAPLUS'~~
ENTER DISPLAY FORMAT (BIB):end

=> d .ca hitstr 15 1-12

L5 ANSWER 1 OF 12 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 2001:139773 HCAPLUS
DOCUMENT NUMBER: 134:237749
TITLE: Design and Synthesis of Inhibitors of Adenosine and AMP Deaminases
AUTHOR(S): Bojack, Guido; Earnshaw, Christopher G.; Klein, Robert; Lindell, Stephen D.; Lowinski, Christian; Preuss, Rainer
CORPORATE SOURCE: Aventis CropScience GmbH, Frankfurt am Main, D-65926, Germany
SOURCE: Organic Letters (2001), 3(6), 839-842
CODEN: ORLEF7; ISSN: 1523-7060
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Nucleosides and nucleotides which are able to undergo covalent hydration in the aglycon ring system are potential inhibitors of the enzymes adenosine deaminase (ADA) and AMP deaminase, resp. Calcns. of the enthalpy of covalent hydration and of enzyme binding energy have been used to design new inhibitors of ADA. The ribosyl triazolotriazine I, which was synthesized as a result of these calcns., exists predominantly as the covalent hydrate II in water and is a potent inhibitor of mammalian ADA (IC50 50 nM). In addn., biol. testing of the I/II mixt. showed that it possessed postemergence herbicidal activity at rates of 320 g ha⁻¹ and below, depending upon the species.

CC 33-9 (Carbohydrates)
Section cross-reference(s): 5, 7
IT 550-33-4, Nebularine 13264-01-2, Deaminoformycin 206450-52-4
254114-35-7 254440-94-3 291536-67-9 330469-91-5
330469-92-6

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study)
 (design and synthesis of C-nucleoside based inhibitors of adenosine and AMP deaminases)

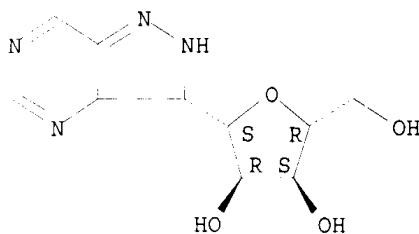
IT 291536-67-9

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study)
 (design and synthesis of C-nucleoside based inhibitors of adenosine and AMP deaminases)

RN 291536-67-9 HCPLUS

CN D-Ribitol, 1,4-anhydro-1-C-2H-pyrazolo[4,3-d]pyrimidin-3-yl-, (1S)- (9CI)
 (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

LS ANSWER 2 OF 12 HCPLUS COPYRIGHT 2002 ACS
 ACCESSION NUMBER: 2000:665549 HCPLUS
 DOCUMENT NUMBER: 133:222974
 TITLE: Preparation of C-nucleosides as adenosine monophosphate deaminase regulators for use in agriculture or medicine
 INVENTOR(S): Bojack, Guido; Lindell, Stephen; Rosinger, Christopher; Dudfield, Philip; Earnshaw, Christopher
 PATENT ASSIGNEE(S): Aventis Cropscience GmbH, Germany
 SOURCE: Ger. Offen., 82 pp.
 CODEN: GWXXBX
 DOCUMENT TYPE: Patent
 LANGUAGE: German
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---------------|--|----------|------------------|----------|
| DE 19912636 | A1 | 20000921 | DE 1999-19912636 | 19990320 |
| WO 2000056734 | A1 | 20000928 | WO 2000-EP2206 | 20000313 |
| W: | AE, AL, AM, AU, AZ, BA, BB, BG, BR, BY, CA, CN, CR, CU, CZ, DM, DZ, EE, GD, GE, HR, HU, ID, IL, IN, IS, JP, KG, KP, KR, KZ, LC, LK, LR, LT, LV, MA, MD, MG, MK, MN, MX, NO, NZ, PL, RO, RU, SG, SI, SK, TJ, TM, TR, TT, UA, UZ, VN, YU, ZA, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM | | | |
| RW: | GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG | | | |
| EP 1165563 | A1 | 20020102 | EP 2000-916932 | 20000313 |
| R: | AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO | | | |

PRIORITY APPLN. INFO.:

DE 1999-19912636 A 19990320
WO 2000-EP2206 W 20000313

OTHER SOURCE(S):

MARPAT 133:222974

AB Title compds. [(I); Q = N, CR1; Q1 = C,N; if Q1 = C, bond Q1-C2 = double; if Q1 = N, bond C2-Q2 = double; Q2 = N, CR2, when Q1 = N, or NR2, O, S, S(O), SO2, when Q1 = C; R = (un)satd. hydrocarbon chain substituted with O, S, NHR4; R1, R2 independently = H, NHR3, OR3, SR3, CN, halogen, N3, NO2, SF5; R3 = H, acyl, (un)satd. (cyclo)alkyl, SO2NH2; R4 = alkyl], useful as herbicides, plant growth regulators, and for the treatment of disease as adenosine monophosphate deaminase or adenosine deaminase regulators, were prep'd. Thus, in four steps, starting from 2',3',5'-tri-O-acetyl-8-aza-9-deaza-inosine, (II) was prep'd. (isolated as the disodium salt). In in vitro adenosine monophosphate deaminase regulation tests in pea plants or calf intestine, II had .gtoreq. 50% inhibition of enzyme activity at 500. μ M. Similar compds. were tested for activity with adenosine deaminase from rabbit muscle, and also proved active.

IC 1CM C07H007-06

ICS C07H023-00; C07H009-04; C07H015-26; C07D487-04; C07D519-00;
A01N043-90; A01N057-16; A01N055-10; A61K031-66; A61K031-695;

A61K031-70

CC 33-9 (Carbohydrates)

Section cross-reference(s): 5, 28, 63

IT 244035-94-7P 254114-35-7P 254440-94-3P 291536-67-9P

291536-68-0P 291536-69-1P 291536-70-4P

291536-71-5P 291536-72-6P

RL BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of C-nucleosides as adenosine monophosphate deaminase regulators for use in agriculture or medicine)

IT 291536-67-9P 291536-69-1P 291536-70-4P

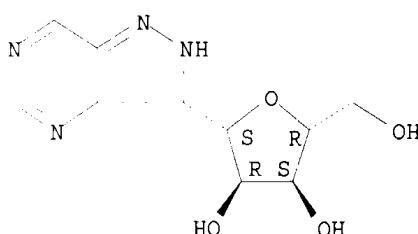
291536-71-5P 291536-72-6P

RL BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of C-nucleosides as adenosine monophosphate deaminase regulators for use in agriculture or medicine)

RN 291536-67-9 HCPLUS

CN D-Ribitol, 1,4-anhydro-1-C-2H-pyrazolo[4,3-d]pyrimidin-3-yl-, (1S)- (9CI)
(CA INDEX NAME)

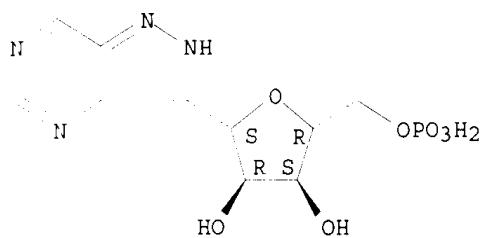
Absolute stereochemistry.



RN 291536-69-1 HCPLUS

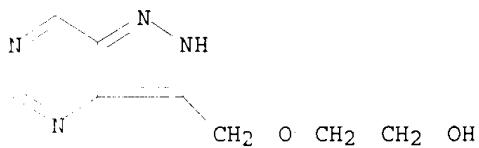
CN D-Ribitol, 1,4-anhydro-1-C-2H-pyrazolo[4,3-d]pyrimidin-3-yl-,
5-(dihydrogen phosphate), disodium salt (9CI) (CA INDEX NAME)

Absolute stereochemistry.

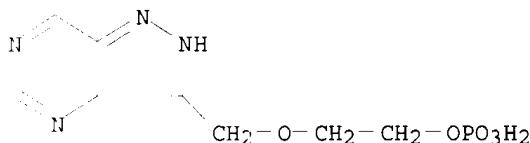


●2 Na

RN 291536-70-4 HCAPLUS
CN Ethanol, 2-(2H-pyrazolo[4,3-d]pyrimidin-3-ylmethoxy)- (9CI) (CA INDEX NAME)



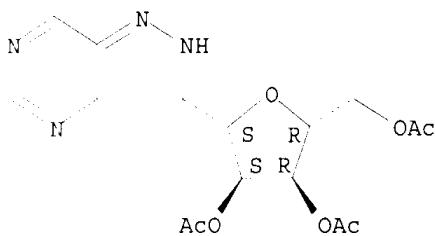
RN 291536-71-5 HCAPLUS
CN Ethanol, 2-(2H-pyrazolo[4,3-d]pyrimidin-3-ylmethoxy)-, dihydrogen phosphate (ester), disodium salt (9CI) (CA INDEX NAME)



●2 Na

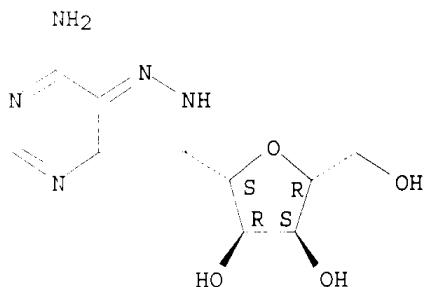
RN 291536-72-6 HCAPLUS
CN D-Ribitol, 1,4-anhydro-1-C-2H-pyrazolo[4,3-d]pyrimidin-3-yl-, 2,3,5-triacetate, (1S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



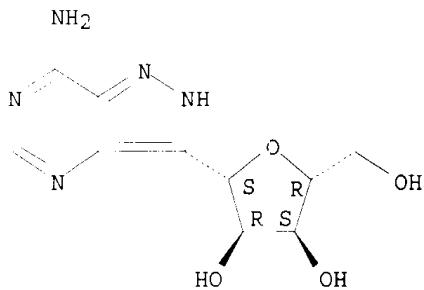
L5 ANSWER 3 OF 12 HCPLUS COPYRIGHT 2002 ACS
 ACCESSION NUMBER: 1994:483847 HCPLUS
 DOCUMENT NUMBER: 121:83847
 TITLE: Tautomerism, protonation, and ionization of formycin in aqueous solution by the pH dependence of ^{13}C chemical shifts and $^{13}\text{C}-\text{H}$ coupling constants
 AUTHOR(S): Cho, Bongsup P.; McGregor, Michael A.
 CORPORATE SOURCE: Coll. Pharm., Univ. Rhode Island, Kingston, RI, 02881, USA
 SOURCE: Nucleosides & Nucleotides (1994), 13(1-3), 481-90
 CODEN: NUNUD5; ISSN: 0732-8311
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB Analyses of the pH dependence of ^{13}C chem. shifts and $^{13}\text{C}-\text{H}$ coupling consts. of formycin in aq. soln. revealed two pKa's, at 4.4 and 9.7, corresponding to a protonation at N4 and an ionization at N1. The N4-protonation results in the transfer of a pyrazolo ring hydrogen from N1 to N2. At physiol. pH, formycin was found to exist as a mix. of N1H and N2H tautomers, with the former being predominant (>94%).
 CC 33-9 (Carbohydrates)
 Section cross-reference(s): 22
 IT 6742-12-7 57101-52-7
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (tautomerism, protonation, and ionization of, in aq. soln.)
 IT 57101-52-7
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (tautomerism, protonation, and ionization of, in aq. soln.)
 RN 57101-52-7 HCPLUS
 CN D-Ribitol, 1-C-(7-amino-2H-pyrazolo[4,3-d]pyrimidin-3-yl)-1,4-anhydro-, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L5 ANSWER 4 OF 12 HCPLUS COPYRIGHT 2002 ACS
 ACCESSION NUMBER: 1990:212992 HCPLUS
 DOCUMENT NUMBER: 112:212992
 TITLE: A quantum chemical study of the enzymic deamination of benzoadenine derivatives. A theoretical model of the interactions occurring between nucleosides and the active site of adenosine deaminase
 AUTHOR(S): Orozco, Modesto; Canela, Enric I.; Franco, Rafael
 CORPORATE SOURCE: Fac. Quim., Univ. Barcelona, Barcelona, E-08028, Spain
 SOURCE: Eur. J. Biochem. (1990), 188(1), 155-63
 CODEN: EJBCAI; ISSN: 0014-2956
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB A theor. study is presented, where, by using both ab initio and semi-empirical methodologies, the properties of benzoadenine derivs. as substrates of adenosine deaminase are discussed. The results suggest that lin-benzoadenine and lin-benzoadenosine can be recognized with an affinity similar to that of adenosine, but only if they are introduced about 0.12 nm deeper inside the active site of the enzyme than the natural substrate adenosine. This fact implies the existence of nonlinear H bonds inside the active site of adenosine deaminase. Ab initio mol. electrostatic potential values suggest that these H bonds can exist, and have stability similar to that of linear H bonds. Finally, the great rate of deamination of lin-benzoadenine, comparable with that of adenosine-despite the absence of the ribose, is explained in the context of the hypothesis that the protonation at the N1 atom is the rate-detg. step of the whole deamination reaction.
 CC 7-4 (Enzymes)
 TT 58-61-7 Adenosine, reactions 69-33-0 73-24-5, Adenine, reactions 6736-58-9, 3-Deazaadenosine 6742-12-7 14432-09-8, 1-Deazaadenosine 53449-12-0, lin-Benzoadenine 53449-43-7, Prox-benzoadenine 53449-44-8, Dist-benzoadenine 57101-52-7 60189-62-0, Lin-Benzoadenosine 60189-88-0 90108-76-2, 1H-Benzimidazo[5,6-g]quinazolin-9-amine 115420-04-7, 4,9-Dihydro-lin-benzoadenine
 RL: RCT (Reactant)
 (reaction of, with adenosine deaminase, quantum chem. study of)
 IT 57101-52-7
 RL: RCT (Reactant)
 (reaction of, with adenosine deaminase, quantum chem. study of)
 RN 57101-52-7 HCPLUS
 CN D-Ribitol, 1-C-(7-amino-2H-pyrazolo[4,3-d]pyrimidin-3-yl)-1,4-anhydro-, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

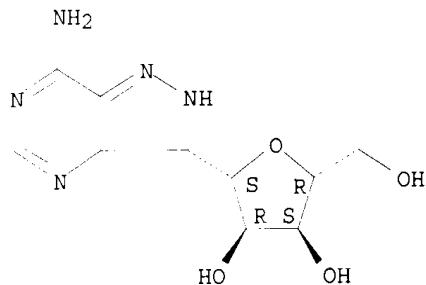


ACCESSION NUMBER: 1989:566765 HCAPLUS
 DOCUMENT NUMBER: 111:166765
 TITLE: Theoretical study of the tautomerism of adenosine and formycin: functional implications
 AUTHOR(S): Orozco, M.; Canela, E. I.; Lluis, C.; Mallol, J.; Franco, R.
 CORPORATE SOURCE: Fac. Quim., Univ. Barcelona, Barcelona, 08028, Spain
 SOURCE: Prog. Clin. Biol. Res. (1989), 291(QSAR: Quant. Struct.-Act. Relat. Drug Des.), 365-8
 CODEN: PCB RD2; ISSN: 0361-7742

DOCUMENT TYPE: Journal
 LANGUAGE: English
 ABSTRACT: The relative energies of amino-imino tautomers of adenosine and N7- and N8-H tautomers of formycin protonated at N1 were calcd. The amino form of adenosine and the N8-H form of formycin were more stable based on data obtained by MNDO, AM 1, and ab initio STO-3G methods. The tautomerism under various reaction conditions may influence nucleoside deamination by adenosine deaminase.

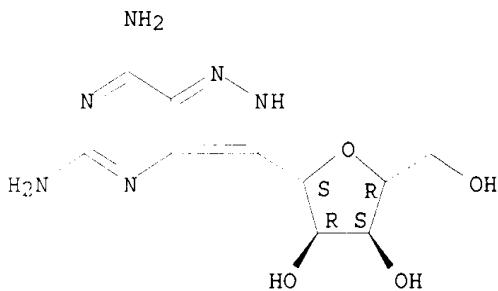
CC 1-3 (Pharmacology)
 IT 58-61-7, Adenosine, biological studies 146-78-1, 2-Fluoroadenosine 2096-10-8, 2-Aminoadenosine 6742-12-7 57101-52-7 82538-40-7
 123162-33-4 123162-34-5 123179-97-5
 123238-52-8
 RL: PRP (Properties)
 (relative energy of, tautomerism and metab. by adenosine deaminase in relation to)
 IT 57101-52-7 123162-33-4 123162-34-5
 123238-52-8
 PT.. PRP (Properties)
 (relative energy of, tautomerism and metab. by adenosine deaminase in relation to)
 RN 57101-52-7 HCAPLUS
 CN D-Ribitol, 1-C-(7-amino-2H-pyrazolo[4,3-d]pyrimidin-3-yl)-1,4-anhydro-, (S) - (9CI) (CA INDEX NAME)

Absolute stereochemistry.



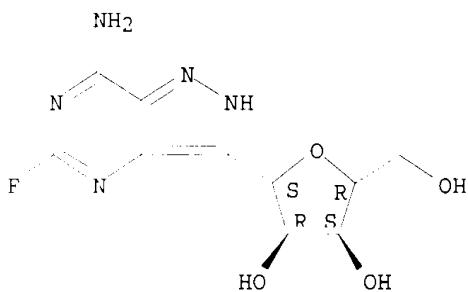
EN 123162-33-4 HCAPLUS
 CN D-Ribitol, 1,4-anhydro-1-C-(5,7-diamino-2H-pyrazolo[4,3-d]pyrimidin-3-yl)-, (1S) - (9CI) (CA INDEX NAME)

Absolute stereochemistry.



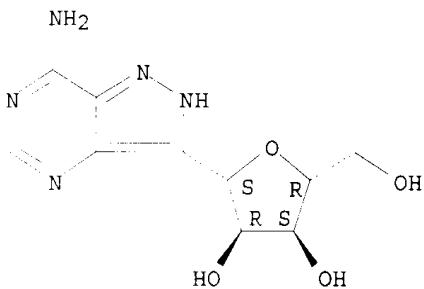
RN 123162-34-5 HCPLUS
CN D-Ribitol, 1-C-(7-amino-5-fluoro-2H-pyrazolo[4,3-d]pyrimidin-3-yl)-1,4-anhydro-, (1S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 123238-52-8 HCPLUS
CN D-Ribitol, 1-C-(7-amino-2H-pyrazolo[4,3-d]pyrimidin-3-yl)-1,4-anhydro-, conjugate monoacid, (1S)- (9CI) (CA INDEX NAME)

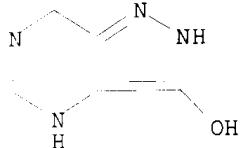
Absolute stereochemistry.



H⁺

L5 ANSWER 6 OF 12 HCPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1983:558362 HCPLUS
DOCUMENT NUMBER: 99:158362

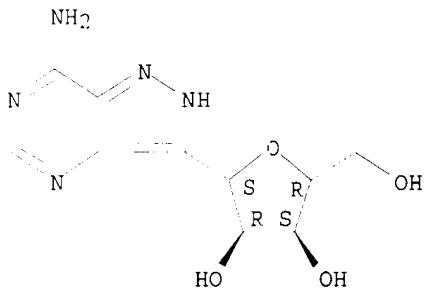
TITLE: Synthesis of 2-substituted 2,6-dihydro-3-hydroxy-7H-pyrazolo[4,3-d]pyrimidin-7-ones
 AUTHOR(S): Ochi, Hisao; Miyasaka, Tadashi
 CORPORATE SOURCE: Sch. Pharm. Sci., Showa Univ., Tokyo, 142, Japan
 SOURCE: Chem. Pharm. Bull. (1983), 31(4), 1228-34
 CODEN: CPBTAL; ISSN: 0009-2363
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 99:158362
 AB Pyrazolo[4,3-d]pyrimidines I (R = Ph, p-tolyl, m-tolyl, 4-ClC₆H₄) were prepd. by redn. of Et 4-nitrosopyrazole-3-carboxylates II (R₁ = NO) and condensation of the resulting II (R₁ = NH₂) with HCONH₂. II (R = NO) were prepd. by nitrosating II (R₁ = H), which were prepd. from Eto₂COCH₂CO₂Et and RNHNH₂.
 CC 28-16 (Heterocyclic Compounds (More Than One Hetero Atom))
 IT 87499-14-7P 87499-15-8P 87499-16-9P 87499-17-0P
 87499-18-1P 87499-19-2P 87499-23-8P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. of)
 IT 87499-14-7P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. of)
 RN 87499-14-7 HCPLUS
 CN 7H-Pyrazolo[4,3-d]pyrimidin-7-one, 2,4-dihydro-3-hydroxy- (9CI) (CA INDEX NAME)



L5 ANSWER 7 OF 12 HCPLUS COPYRIGHT 2002 ACS
 ACCESSION NUMBER: 1980:513653 HCPLUS
 DOCUMENT NUMBER: 93:113653
 TITLE: Tautomerism of formycin. Mechanism of interconversion
 AUTHOR(S): Dodin, Guy; Bensaude, Olivier; Dubois, Jacques Emile
 CORPORATE SOURCE: Inst. Topol., Univ. Paris, Paris, 75005, Fr.
 SOURCE: J. Am. Chem. Soc. (1980), 102(11), 3897-9
 CODEN: JACSAT; ISSN: 0002-7863
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB The tautomeric equil. between 1H- and 2H-formycin (7-amino-3.β-D-ribofuranosyl-1H-pyrazolo[4,3-d]pyrimidine) has a const. KT = N(2)H/N(1)H = 0.2 and an enthalpy estd. as 1 kcal mol⁻¹. The tautomeric interconversion is catalyzed by H⁺ (kH⁺ = 3 .times. 109 M⁻¹ s⁻¹) and by OH⁻ (kOH = 5 .times. 109 M⁻¹ s⁻¹). No other catalytic pathway such as water catalysis or tautomerization via tautomeric cations contributes significantly to the interconversion. Protonation of formycin does not occur significantly on the pyrazole ring.
 CC 22-6 (Physical Organic Chemistry)
 IT 6742-12-7 57101-52-7
 RL: RCT (Reactant)
 (tautomerization of, kinetics and thermodn. of)

IT 57101-52-7
 RL: RCT (Reactant)
 (tautomerization of, kinetics and thermodn. of)
 RN 57101-52-7 HCPLUS
 CN D-Ribitol, 1-C-(7-amino-2H-pyrazolo[4,3-d]pyrimidin-3-yl)-1,4-anhydro-,
 (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L5 ANSWER 8 OF 12 HCPLUS COPYRIGHT 2002 ACS
 ACCESSION NUMBER: 1979:611773 HCPLUS
 DOCUMENT NUMBER: 91:211773
 TITLE: Formycin 3',5'-cyclic phosphate
 INVENTOR(S): Umezawa, Sumio; Umezawa, Hamao; Kawamura, Kenji;
 Makabe, Osamu
 PATENT ASSIGNEE(S): Meiji Seika Kaisha, Ltd., Japan
 SOURCE: Jpn. Kokai Tokkyo Koho, 6 pp.
 CODEN: JKXXAF
 DOCUMENT TYPE: Patent
 LANGUAGE: Japanese
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

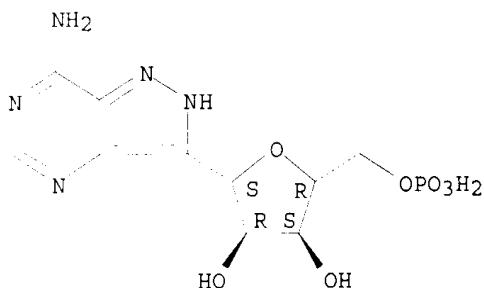
| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|-------------|------|----------|-----------------|----------|
| JP 54088295 | A2 | 19790713 | JP 1977-154396 | 19771223 |
| JP 61002072 | B4 | 19860122 | | |

AB A mixt. of 4.5 mL (MeO)₃PO, 0.6 mL POCl₃, and 1 g formycin was stirred 2 h at -5.degree. and treated with Dowex 50W .times. 8 (H⁺) to give 845 mg formycin-5'-phosphate (I). Dicyclohexylcarbodiimide (1.65 g) in pyridine was added to a refluxing mixt. of 1.46 g I and 200 mL (Me₂N)₃PO in pyridine over 1 h, the whole refluxed 1 h, allowed to stand overnight at room temp., stirred with H₂O at room temp., and treated with Dowex 50W .times. 8 (H⁺) to give 41% II (R = H). II (R = Me, Me₂CH) were also prepd.

IC C07H007-06
 CC 33-7 (Carbohydrates)
 IT 71972-00-4P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
 (prep. and cyclization of)
 IT 67187-18-2P 71972-01-5P 71972-02-6P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (prep. of)
 IT 71972-00-4P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
 (prep. and cyclization of)

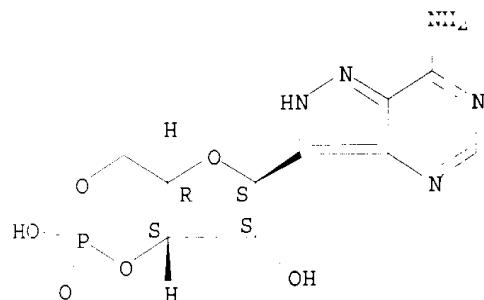
RN 71972-00-4 HCPLUS
 CN D-Ribitol, 1-C-(7-amino-2H-pyrazolo[4,3-d]pyrimidin-3-yl)-1,4-anhydro-,
 5-(dihydrogen phosphate), (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 71972-01-5P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (prep. of)
 RN 71972-01-5 HCPLUS
 CN D-Ribitol, 1-C-(7-amino-2H-pyrazolo[4,3-d]pyrimidin-3-yl)-1,4-anhydro-,
 cyclic 3,5-(hydrogen phosphate), (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L5 ANSWER 9 OF 12 HCPLUS COPYRIGHT 2002 ACS
 ACCESSION NUMBER: 1978:597857 HCPLUS
 DOCUMENT NUMBER: 89:197857
 TITLE: Synthesis of pyrazoles. A simple preparative synthesis of C-nucleosidic antibiotics formycin and formycin B
 AUTHOR(S): Kalvoda, Ladislav
 CORPORATE SOURCE: Inst. Org. Chem. Biochem., Czech. Acad. Sci., Prague,
 Czech.
 SOURCE: Collect. Czech. Chem. Commun. (1978), 43(5), 1431-7
 CODEN: CCCCAK; ISSN: 0366-547X
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB Formycin (I, R1 = H) and formycin B (II, R1 = H) were synthesized by a route based on cycloaddn. of N2CHR2 to NCCR3:CHCO2R4 with elimination of HCN yielding pyrazoles III. Thus, 3,4,6-tri-O-benzoyl-2,5-anhydro-D-allonic acid was converted with SOCl2 to chloride and treated with Ph3P:CHCO2CMe3 in the presence of HCN to yield 60% tert-Bu

(Z)-3-cyano-3-(2,3,5-tri-O-benzoyl-.beta.-D-ribofuranosyl)propenoate, which was treated with N₂CHCN or N₂CHCO₂Et to give, resp., 86% IV (R₅ = CO₂CMe₃, R₆ = CN) (V) and 73% IV (R₅ = CO₂CMe₃, R₆ = CO₂Et) (VI). The CMe₃ group of V was split off with HCO₂H at 60-70.degree. and the acid was heated with NET₃, Cl₃CCH₂OH, and (PhO)₂P(O)N₃ in PhMe 5 h at 100.degree. to yield 36% IV (R₅ = NHCO₂CH₂CCl₃, R₆ = CN). The CH₂CCl₃ group was cleaved with Zn dust and NH₄Cl in boiling MeOH and the product was cyclized by heating with HN:CHNH₂ to yield 29.5% I (R₁ = Bz) (VII). Analogously, VI gave 58% IV (R₅ = NHCO₂CH₂CCl₃, R₆ = CO₂Et) which yielded 67% II (R₁ = Bz) (VIII). Methanolysis of VII and VIII gave 90% formycin and 95% formycin B, identical with natural antibiotics prepd. by fermn.

CC 33-7 (Carbohydrates)

Section cross-reference(s): 28

IT 67560-80-9P 67560-82-1P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation) (prepn. and methanolysis of)

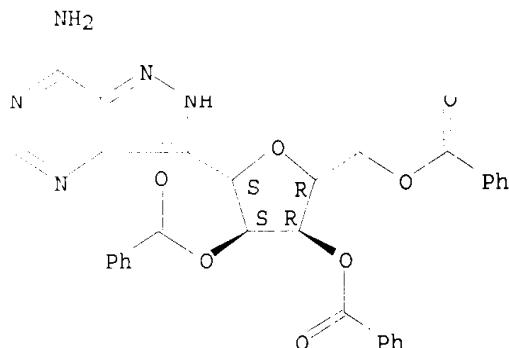
IT 67560-80-9P 67560-82-1P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation) (prepn. and methanolysis of)

RN 67560-80-9 HCPLUS

CN D-Ribitol, 1-C-(7-amino-2H-pyrazolo[4,3-d]pyrimidin-3-yl)-1,4-anhydro-, 2,3,5-tribenzoate, (S)- (9CI) (CA INDEX NAME)

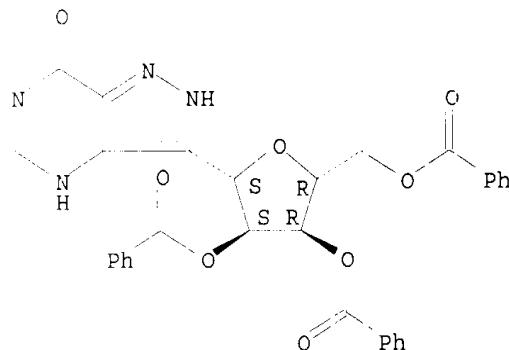
Absolute stereochemistry.



RN 67560-82-1 HCPLUS

CN 7H-Pyrazolo[4,3-d]pyrimidin-7-one, 2,4-dihydro-3-(2,3,5-tri-O-benzoyl-.beta.-D-ribofuranosyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L5 ANSWER 10 OF 12 HCAPLUS COPYRIGHT 2002 ACS
 ACCESSION NUMBER: 1978:510233 HCAPLUS
 DOCUMENT NUMBER: 89:110233
 TITLE: Dynamics of tautomerization of formycin
 AUTHOR(S): Cole, Francis X.; Schimmel, Paul R.
 CORPORATE SOURCE: Dep. Biol., Massachusetts Inst. Technol., Cambridge,
 Mass., USA
 SOURCE: J. Am. Chem. Soc. (1978), 100(12), 3957-8
 CODEN: JACSAT; ISSN: 0002-7863

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The dynamics of tautomerization of formycin A was investigated by the temp.-jump method. The tautomerization between 1-H- and 2-H-formycin was followed spectrophotometrically. In unbuffered solns., the tautomerization is characterized by a single relaxation process with a time const. of around 10-4 sec at 25.degree.. The relaxation time is pH dependent, being faster at acid pH values. The rate of tautomerization of neutral formycin is 3.4 times 103 sec-1 (25.degree.) and over 10-fold more rapid for the protonated form. Basic species such as unprotonated imidazole greatly accelerate the rate of tautomerization. The rate detg. step in tautomerization is abstraction by a basic species of a proton from N-1 (or N-2) in the pyrazole part of the ring; the transient intermediate then quickly adds back a proton from the solvent or a protonated base.

C1 33-7 (Carbohydrates)

Section cross-reference(s): 22, 28

IT 57101-52-7P

PL: FORM (Formation, nonpreparative); PREP (Preparation)
 (formation or, by tautomerization)

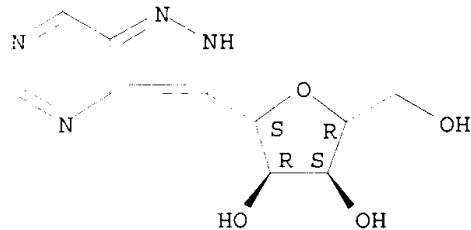
IT 57101-52-7P

PL: FORM (Formation, nonpreparative); PREP (Preparation)
 (formation of, by tautomerization)

RN 57101-52-7 HCAPLUS

CN D-Ribitol, 1-C-(7-amino-2H-pyrazolo[4,3-d]pyrimidin-3-yl)-1,4-anhydro-,
 (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

NH₂

L5 ANSWER 11 OF 12 HCAPLUS COPYRIGHT 2002 ACS
 ACCESSION NUMBER: 1977:468560 HCAPLUS
 DOCUMENT NUMBER: 87:68560
 TITLE: Fluorescent derivatives of nucleosides
 AUTHOR(S): Chung, Hsiao L.; Zemlicka, Jiri
 CORPORATE SOURCE: Michigan Cancer Found., Detroit, Mich., USA
 SOURCE: J. Heterocycl. Chem. (1977), 14(1), 135-8

CODEN: JHTCAD

DOCUMENT TYPE:

Journal

LANGUAGE:

English

AB In this abstract, R₁ = .beta.-D-ribofuranosyl. The fluorescence spectra of anhydro- (I, II and III) and methylenerebonucleosides (IV, V, VI (Q = N, R = H, Br; Q = CH, R = H), and VII were related to the known fluorescent formycin. The aminomethylene group in IV-VII leads to fluorescence but causes bathochromic shifts. I and II fluoresce more strongly than formycin, and show the bathochromic shift.

CC 33-7 (Carbohydrates)

Section cross-reference(s): 22, 28

IT 17331-14-5 17331-15-6 17331-16-7 57101-52-7 57553-78-3

57573-29-2 57573-30-5 57881-18-2 57881-19-3 63347-44-4

63358-78-1

RL: PRP (Properties)

(fluorescence spectrum of)

IT 57101-52-7 63347-44-4 63358-78-1

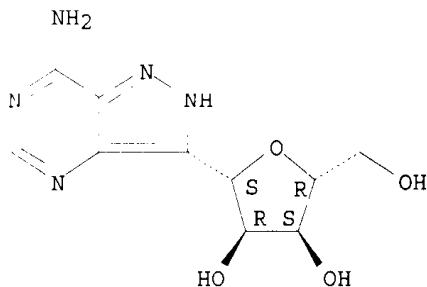
RL: PRP (Properties)

(fluorescence spectrum of)

PN 57101-52-7 HCPLUS

CN D-Ribitol, 1-C-(7-amino-2H-pyrazolo[4,3-d]pyrimidin-3-yl)-1,4-anhydro-, (S)- (9CI) (CA INDEX NAME)

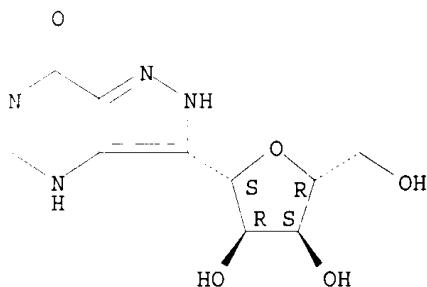
Absolute stereochemistry.



PN 63347-44-4 HCPLUS

CN 7H-Pyrazolo[4,3-d]pyrimidin-7-one, 2,4-dihydro-3-.beta.-D-ribofuranosyl- (9CI) (CA INDEX NAME)

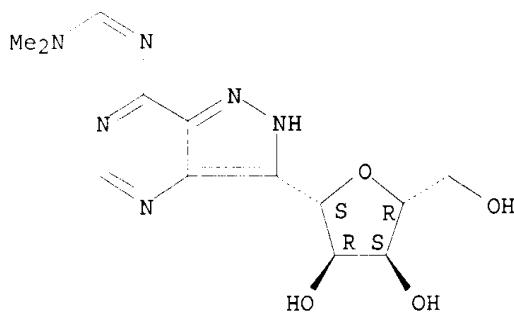
Absolute stereochemistry.



EN 63358-78-1 HCPLUS

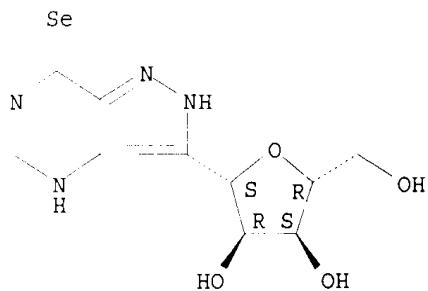
CN Methanimidamide, N,N-dimethyl-N'-(3-.beta.-D-ribofuranosyl-2H-pyrazolo[4,3-d]pyrimidin-7-yl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.



L5 ANSWER 12 OF 12 HCAPLUS COPYRIGHT 2002 ACS
 ACCESSION NUMBER: 1975:497797 HCAPLUS
 DOCUMENT NUMBER: 83:97797
 TITLE: Novel synthesis of 6-seleno-substituted nucleosides,
 nucleotides, and cyclic nucleotides
 AUTHOP (S): Shieh, Chyng-Yann; Chu, Shih-Hsi
 CORPOFATE SOURCE: Div. Biol. Med. Sci., Brown Univ., Providence, R. I.,
 USA
 SOURCE: J. Chem. Soc., Chem. Commun. (1975), (9), 319-20
 CODEN: JCCCAT
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB Treatment of the amino heterocycles I (X = CH, X1 = N, R = R1 = H, R2 = beta.-D-ribofuranosyl, 3',4'-cyclic phosphoribosyl, arabinofuranosyl; X = CH, X1 = N, R2 = 3',5'-cyclic phosphoribosyl, 5'-phosphoribosyl; X = NH, X1 = C, R = R1 = H, R2 = .beta.-D-ribofuranosyl) with excess H2Se in pyridine-H2O in a sealed tube at 65.degree. gave 21-75% of the title compds. II. Thus, treatment of I (X = CH, X1 = N, R = R1 = H, R2 = .beta.-D-ribofuranosyl) for 5 days gave 56% of the corresponding Se compd.
 CC 33-7 (Carbohydrates)
 IT 29411-74-3P 40093-99-0P 56477-08-8P 56477-11-3P 56477-14-6P
 56477-16-8P 57101-53-8P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. of)
 IT 58-61-7, reactions 60-92-4 2096-10-8 5536-17-4 10254-91-8
 50884-82-7 57101-52-7
 FL: RCT (Reactant)
 (substitution reaction with hydrogen selenide)
 IT 57101-53-8P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. of)
 RN 57101-53-8 HCAPLUS
 CN 7H-Pyrazolo[4,3-d]pyrimidine-7-selone, 2,4-dihydro-3-.beta.-D-ribofuranosyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 57101-52-7

RL: RCT (Reactant)

(substitution reaction with hydrogen selenide)

RN 57101-52-7 HCAPLUS

CN D-Ribitol, 1-C-(7-amino-2H-pyrazolo[4,3-d]pyrimidin-3-yl)-1,4-anhydro-,
(S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

